

Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016675.D
 Acq On : 02 Oct 2021 17:45
 Operator : CG/JU
 Sample : PB139275BS
 Misc :
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 PB139275BS

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 1 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BN016675.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.253	16	19	21	rBV	8996	12686	2.61%	0.159%
2	3.290	21	23	43	rVB	5328	25689	5.29%	0.321%
3	3.576	51	54	55	rBV	5895	8050	1.66%	0.101%
4	6.822	401	406	418	rBV	25268	65130	13.42%	0.815%
5	6.978	418	423	429	rVV	17779	39738	8.19%	0.497%
6	7.080	429	434	440	rVV	37829	78373	16.15%	0.981%
7	7.200	440	447	460	rVB	12792	35187	7.25%	0.440%
8	7.523	478	482	489	rVB	7331	16381	3.38%	0.205%
9	7.642	490	495	508	rVB2	52951	129822	26.75%	1.624%
10	7.956	524	529	539	rVB2	51352	116882	24.09%	1.462%
11	8.168	547	552	557	rBV	3378	8135	1.68%	0.102%
12	8.430	571	577	591	rBV3	22377	53461	11.02%	0.669%
13	8.696	594	598	601	rBV	5166	9680	1.99%	0.121%
14	8.784	601	605	606	rBV	35931	66947	13.80%	0.838%
15	8.822	606	608	616	rVB	29415	55273	11.39%	0.692%
16	9.342	645	649	656	rBV	50108	83836	17.28%	1.049%
17	9.532	660	664	666	rVV	3271	7013	1.45%	0.088%
18	9.596	666	669	684	rVV	9334	17371	3.58%	0.217%
19	9.836	685	688	702	rVV	16719	30051	6.19%	0.376%
20	10.052	702	705	715	rVB	4101	9352	1.93%	0.117%
21	10.407	729	733	735	rBV	113557	208631	43.00%	2.610%
22	10.457	735	737	741	rVV	114583	190403	39.24%	2.382%
23	10.571	743	746	756	rVV	29470	64911	13.38%	0.812%
24	10.749	756	760	763	rVB	34829	59951	12.36%	0.750%
25	11.306	801	804	811	rBV	1925	4999	1.03%	0.063%
26	11.709	854	865	894	rBV	13487	26263	5.41%	0.329%
27	12.003	921	931	939	rBV	60826	98523	20.30%	1.233%
28	12.078	939	948	972	rVV	133440	219735	45.28%	2.749%
29	12.296	987	997	1021	rVV	132162	211941	43.68%	2.652%
30	12.695	1056	1059	1062	rBV	17404	29290	6.04%	0.366%
31	12.759	1062	1064	1071	rVB	12159	25220	5.20%	0.316%
32	12.886	1071	1074	1078	rBV	127257	208514	42.97%	2.609%
33	13.140	1090	1094	1097	rBV	79569	135698	27.97%	1.698%
34	13.736	1138	1141	1143	rBV	12320	17500	3.61%	0.219%
35	13.850	1147	1150	1153	rVB	19909	28464	5.87%	0.356%
36	13.939	1155	1157	1158	rBV	5346	8675	1.79%	0.109%

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Sampling : 1

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Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

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37	13.990	1158	1161	1164	rVB	96378	160380	33.05%	2.007%
38	14.269	1180	1183	1185	rBV	143713	206180	42.49%	2.580%
39	14.332	1185	1188	1191	rVB	178578	256373	52.84%	3.207%
40	14.649	1209	1213	1220	rBV3	15964	44123	9.09%	0.552%
41	14.814	1224	1226	1230	rVV	5299	9489	1.96%	0.119%
42	14.903	1230	1233	1243	rVB	7711	12953	2.67%	0.162%
43	15.106	1246	1249	1252	rBV	8990	11690	2.41%	0.146%
44	15.322	1263	1266	1270	rBV2	236314	365024	75.23%	4.567%
45	15.411	1270	1273	1280	rVV2	2779	8059	1.66%	0.101%
46	15.537	1280	1283	1287	rVV	37443	64847	13.36%	0.811%
47	15.614	1287	1289	1298	rVV2	42387	66502	13.71%	0.832%
48	15.766	1298	1301	1311	rVB2	13442	22591	4.66%	0.283%
49	16.226	1334	1338	1341	rBV2	61246	93568	19.28%	1.171%
50	16.324	1343	1346	1350	rVB	49392	75239	15.51%	0.941%
51	16.506	1358	1361	1372	rBV	20712	34385	7.09%	0.430%
52	16.677	1372	1375	1384	rBV	19203	34256	7.06%	0.429%
53	17.018	1400	1403	1405	rBV	98342	165911	34.19%	2.076%
54	17.066	1405	1407	1410	rVV	154153	223741	46.11%	2.799%
55	17.151	1411	1414	1434	rVB	111858	189743	39.10%	2.374%
56	17.431	1434	1437	1453	rBV	85802	139873	28.83%	1.750%
57	18.015	1482	1485	1515	rVB	5525	7602	1.57%	0.095%
58	19.063	1686	1696	1699	rBV	118907	164945	33.99%	2.064%
59	19.098	1699	1703	1742	rVB	191937	271471	55.95%	3.396%
60	19.460	1767	1776	1813	rBV	193218	267109	55.05%	3.342%
61	19.678	1813	1820	1858	rVB	111911	144833	29.85%	1.812%
62	20.378	1918	1921	1924	rBV	48727	58835	12.13%	0.736%
63	21.164	1993	1995	1997	rBV	49639	62778	12.94%	0.785%
64	21.217	1997	2000	2003	rVV2	206235	429153	88.44%	5.369%
65	21.270	2003	2005	2017	rVB	204022	281126	57.94%	3.517%
66	22.056	2076	2079	2082	rBV	71030	88945	18.33%	1.113%
67	22.807	2216	2229	2235	rBV	125791	212867	43.87%	2.663%
68	22.851	2235	2242	2304	rVB	136548	260166	53.62%	3.255%
69	23.382	2384	2397	2415	rBV	84791	191546	39.48%	2.396%
70	23.484	2416	2427	2497	rVB	98290	217748	44.88%	2.724%
71	24.083	2593	2602	2620	rBV	5193	10258	2.11%	0.128%
72	24.857	2816	2828	2844	rBV2	5598	12548	2.59%	0.157%
73	25.774	3068	3096	3176	rBV3	118349	485232	100.00%	6.071%
74	26.456	3273	3295	3368	rBV	67408	228165	47.02%	2.855%
75	26.825	3390	3403	3438	rVB	1388	4932	1.02%	0.062%

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Integration Parameters: rteint.p
Integrator: RTE
Smoothing : OFF Filtering: 5
Sampling : 1 Min Area: 1 % of largest Peak
Start Thrs: 0.2 Max Peaks: 100
Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

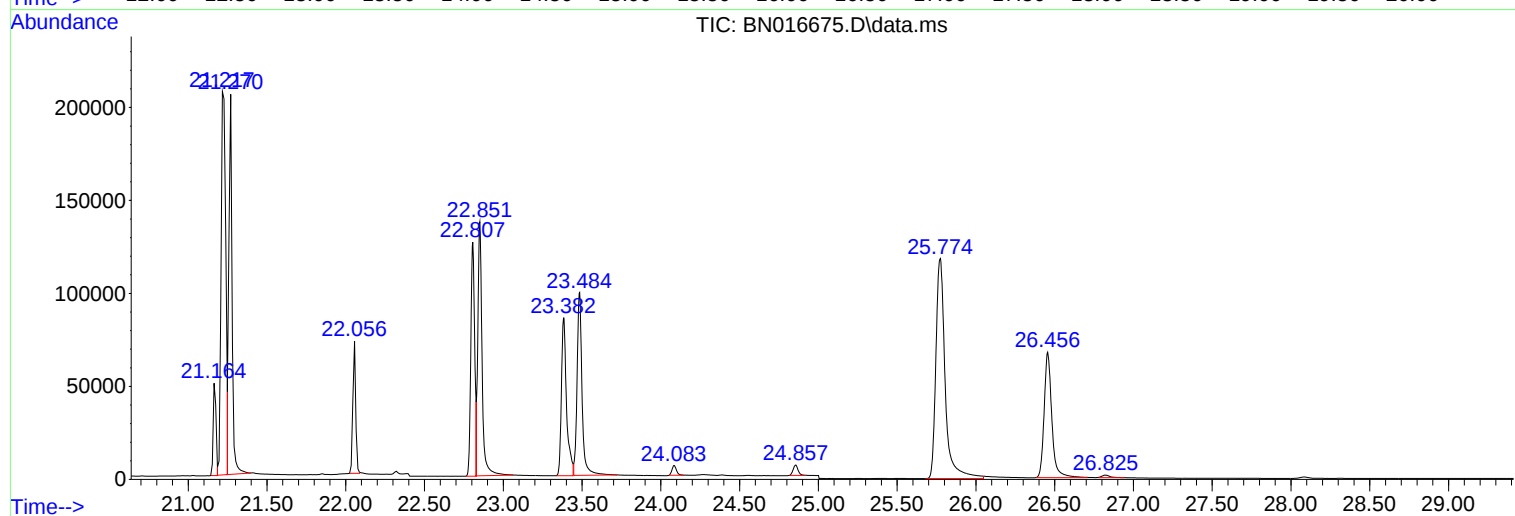
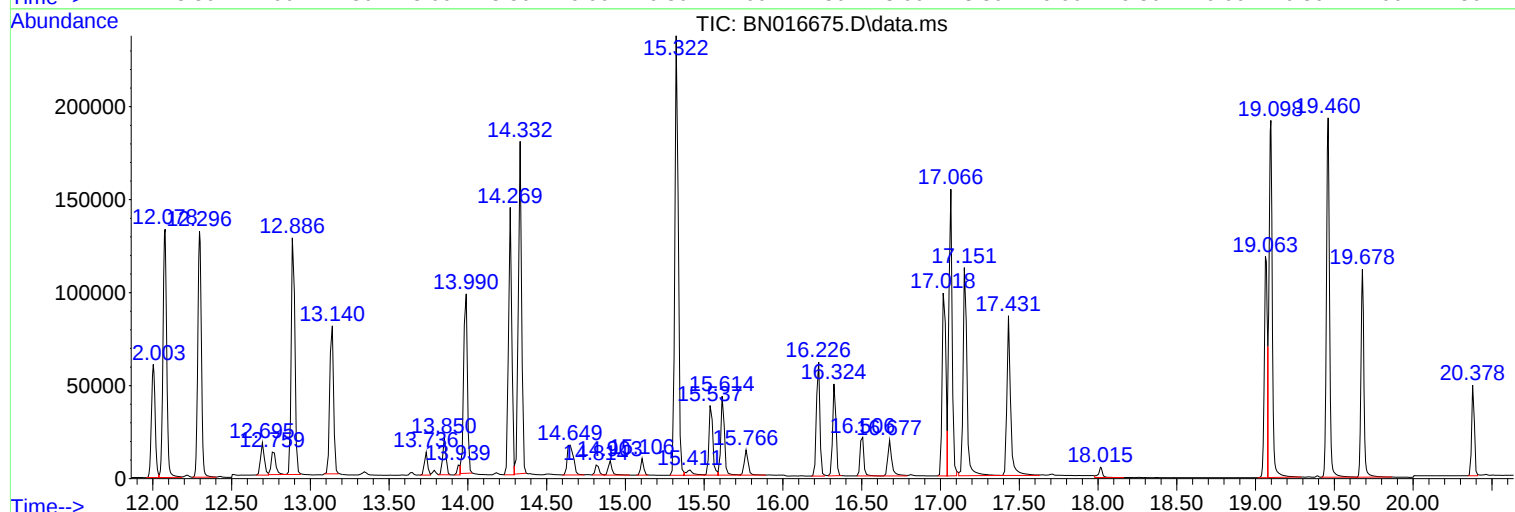
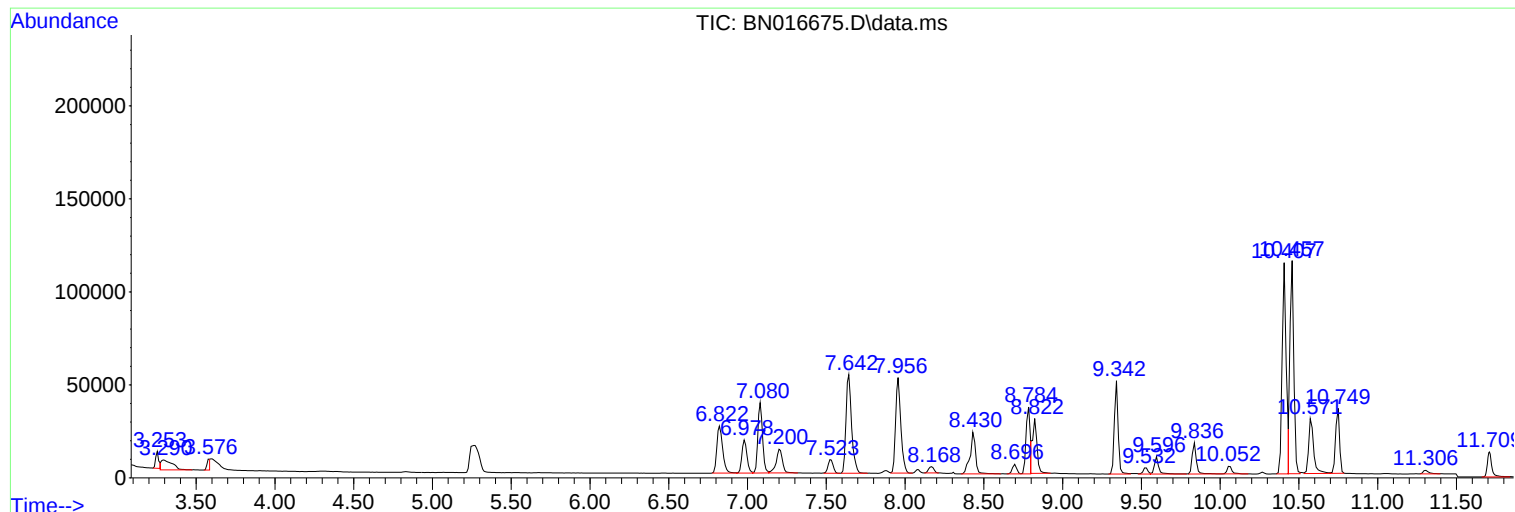
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Instrument :
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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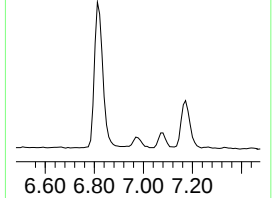
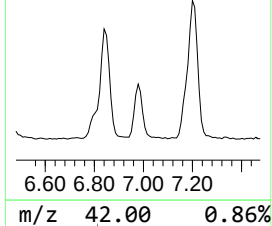
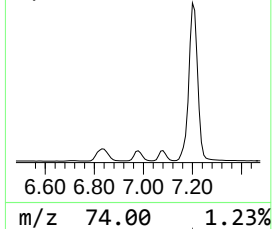
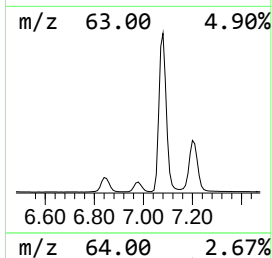
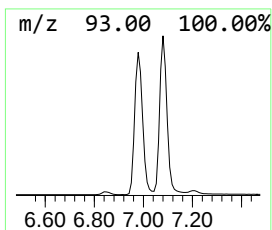
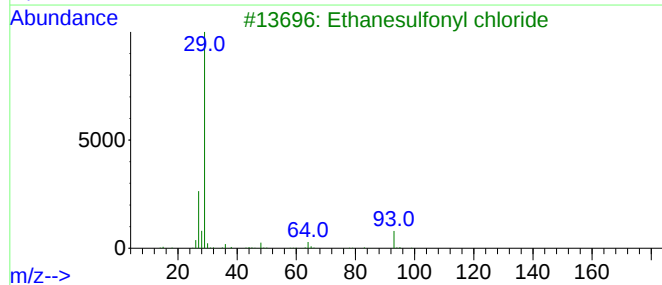
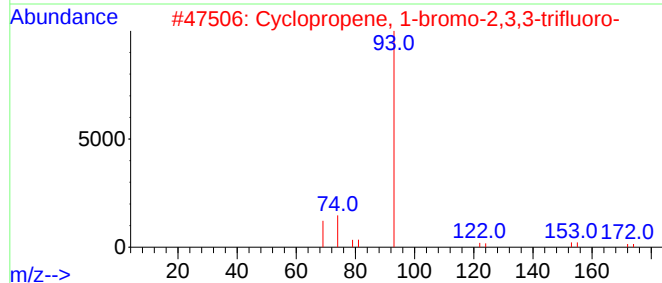
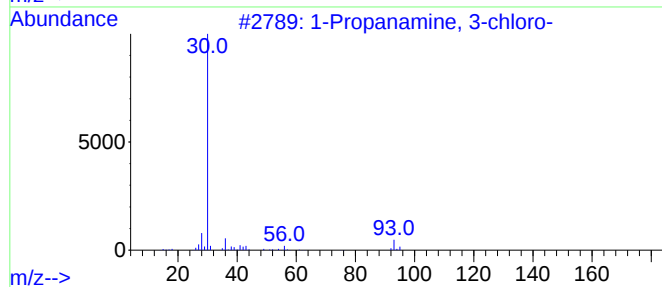
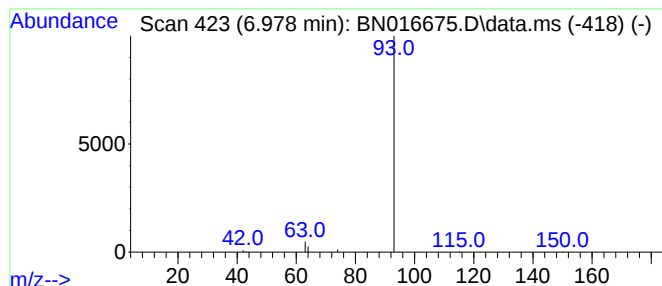
Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 1-Propanamine, 3-chloro- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.978	0.12 ng	39738	1,4-Dichlorobenzene-d4	7.642

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Propanamine, 3-chloro-	93	C3H8ClN	014753-26-5	1
2		Cyclopropene, 1-bromo-2,3,3-trif...	172	C3BrF3	029777-44-4	1
3		Ethanesulfonyl chloride	128	C2H5ClO2S	000594-44-5	1
4		Carbonochloridic acid, ethyl ester	108	C3H5ClO2	000541-41-3	1
5		Ethenesulfonyl chloride	126	C2H3ClO2S	006608-47-5	1



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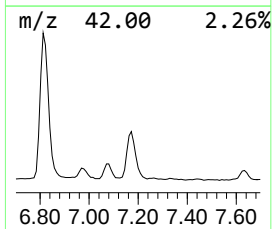
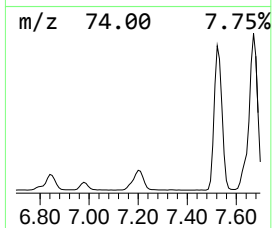
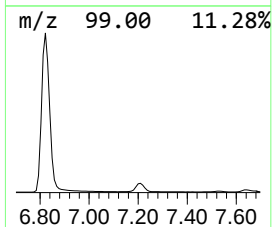
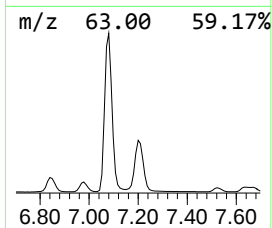
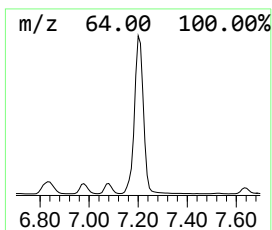
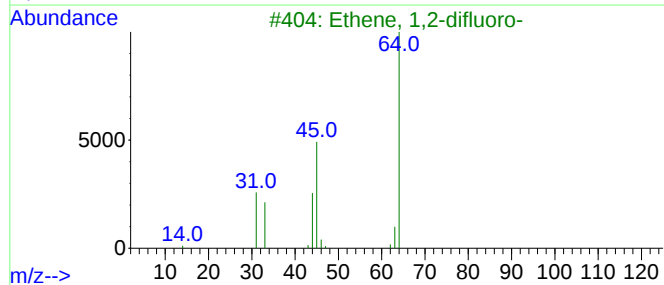
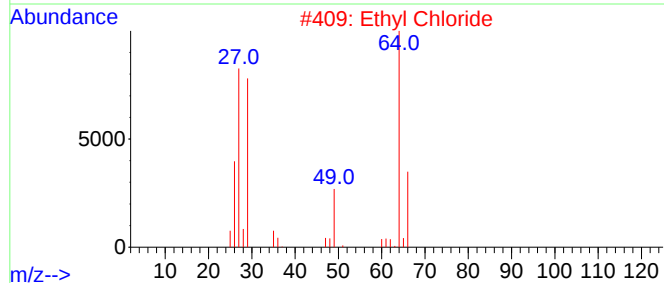
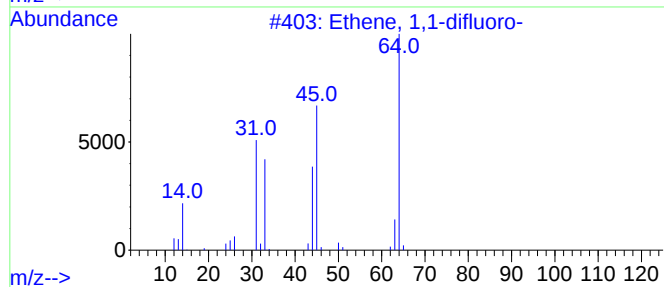
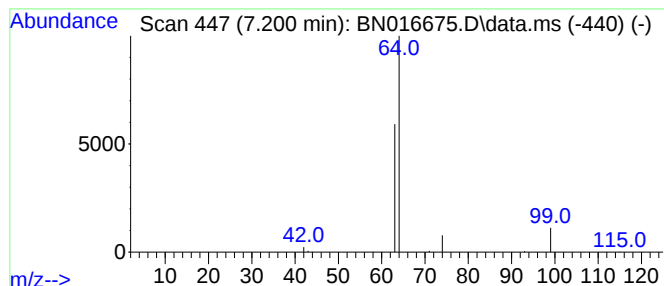
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Ethene, 1,1-difluoro- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.200	0.11 ng	35187	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	3
2			Ethyl Chloride	64	C2H5Cl	000075-00-3	3
3			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	3
4			Sulfur dioxide	64	O2S	007446-09-5	3
5			(S)-(-)-2-Chloropropionic acid	108	C3H5ClO2	029617-66-1	2



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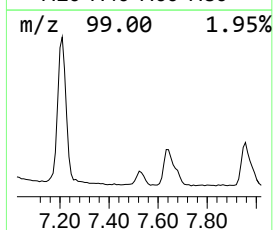
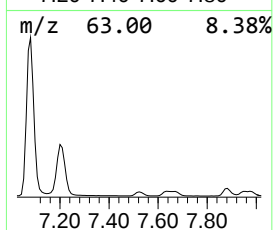
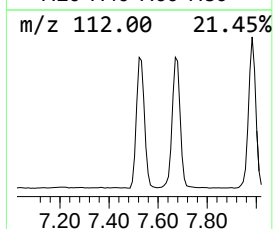
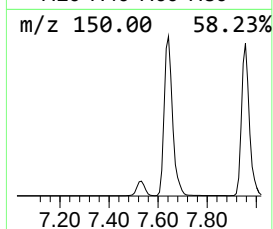
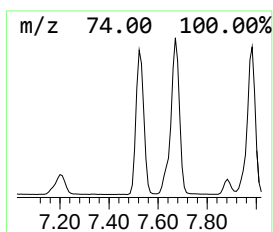
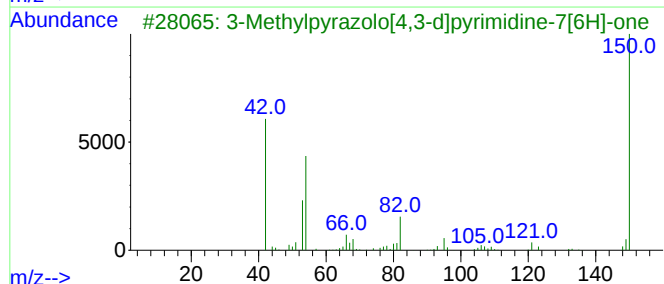
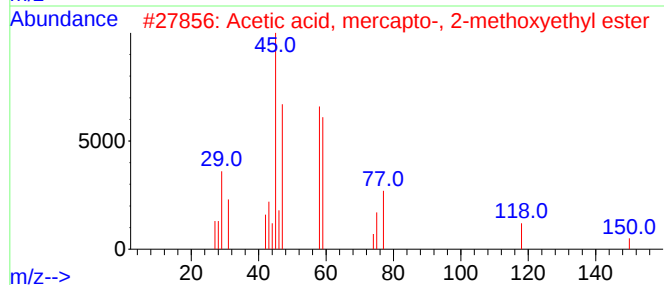
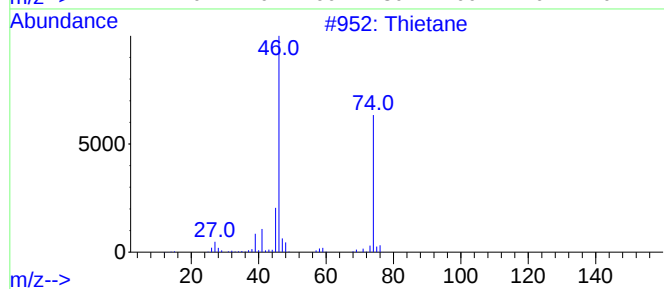
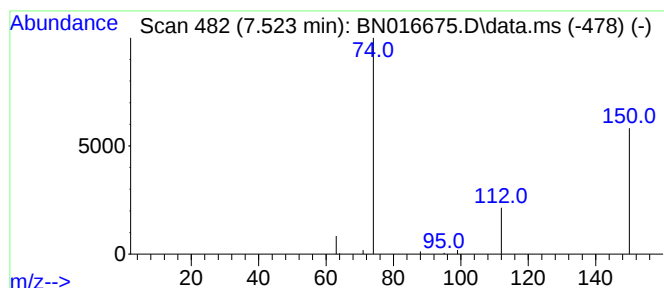
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Thietane Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.523	0.05 ng	16381	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Thietane	74	C3H6S	000287-27-4	3
2			Acetic acid, mercapto-, 2-methox...	150	C5H10O3S	019788-48-8	3
3			3-Methylpyrazolo[4,3-d]pyrimidin...	150	C6H6N4O	005399-94-0	2
4			3-Cyano-2,6-dihydroxy-4-methylpy...	150	C7H6N2O2	005444-02-0	2
5			3-Methyl-4,4'-bi(1,2,4-triazole)	150	C5H6N6	063523-91-1	2



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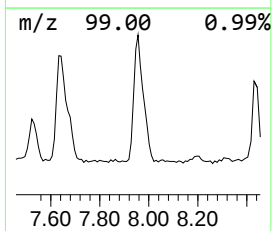
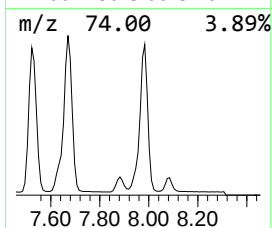
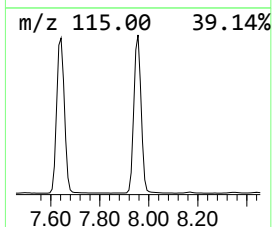
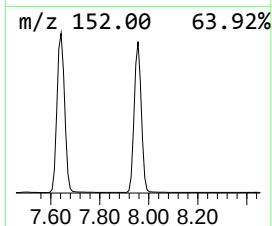
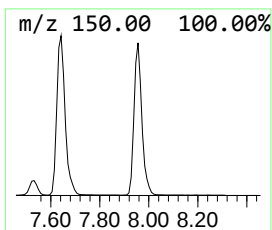
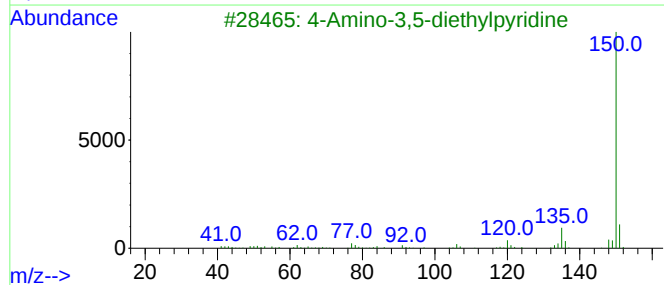
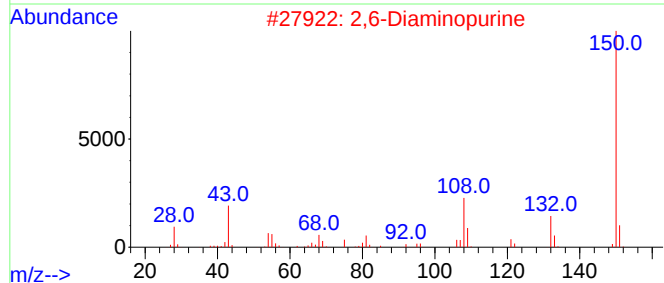
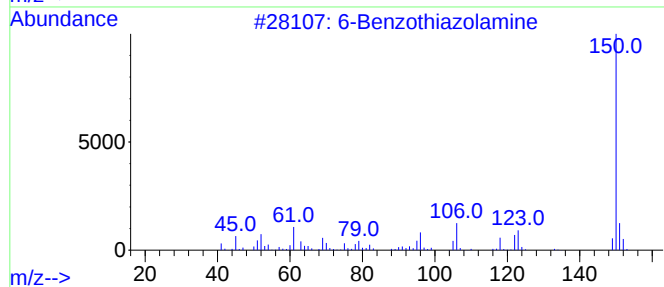
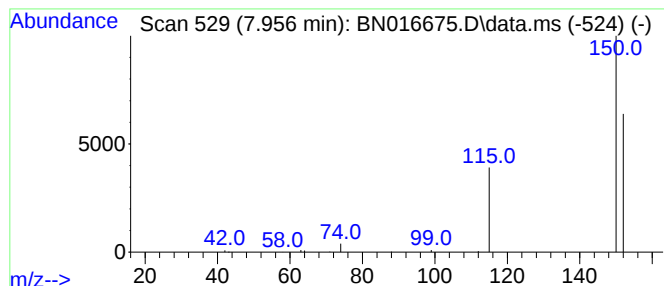
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 6-Benzothiazolamine Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.956	0.36 ng	116882	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			6-Benzothiazolamine	150	C7H6N2S	000533-30-2	4
2			2,6-Diaminopurine	150	C5H6N6	001904-98-9	2
3			4-Amino-3,5-diethylpyridine	150	C9H14N2	1000128-75-1	2
4			Benzene, 1,2,3,4-tetrafluoro-	150	C6H2F4	000551-62-2	2
5			2-Benzimidazolethiol	150	C7H6N2S	000583-39-1	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016675.D
Acq On : 02 Oct 2021 17:45
Operator : CG/JU
Sample : PB139275BS
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139275BS

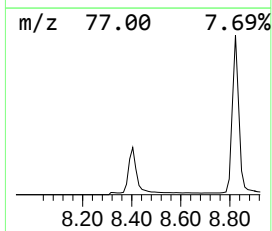
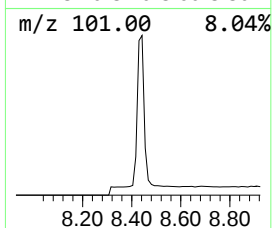
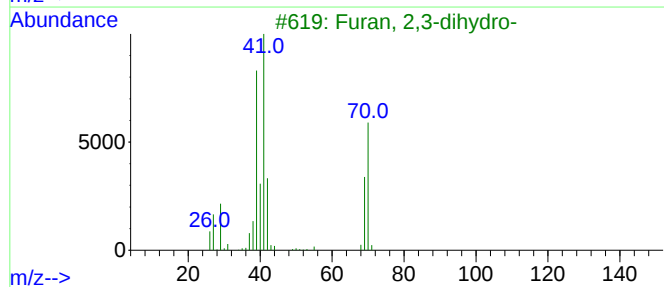
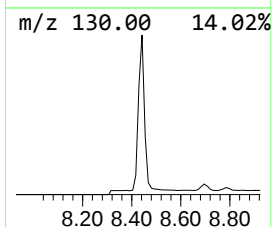
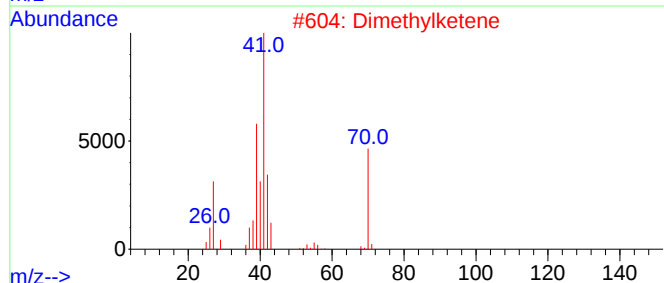
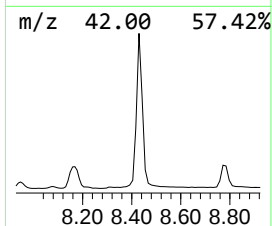
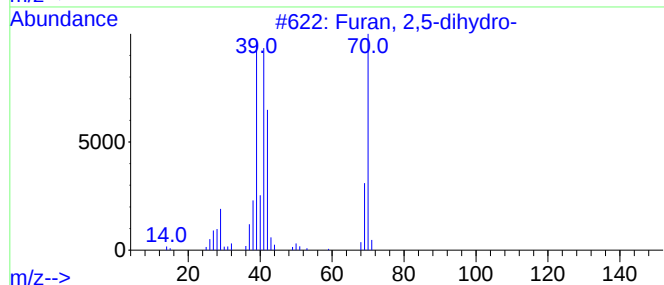
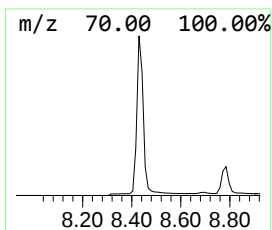
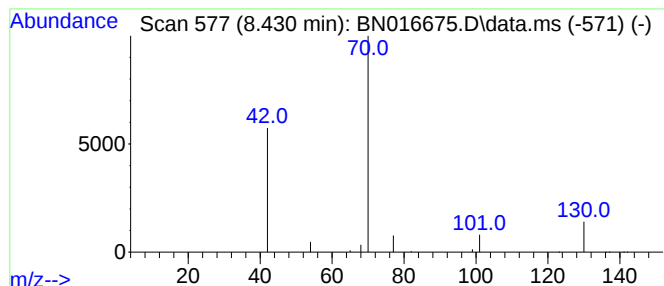
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Furan, 2,5-dihydro- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.430	0.16 ng	53461	1,4-Dichlorobenzene-d4	7.642

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	7
2			Dimethylketene	70	C4H6O	000598-26-5	5
3			Furan, 2,3-dihydro-	70	C4H6O	001191-99-7	5
4			1-Oxa-3,4-diazacyclopentadiene	70	C2H2N2O	000288-99-3	4
5			1-Propanamine, N-nitroso-N-propyl-	130	C6H14N2O	000621-64-7	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016675.D
Acq On : 02 Oct 2021 17:45
Operator : CG/JU
Sample : PB139275BS
Misc :
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Instrument :
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ClientSampleId :
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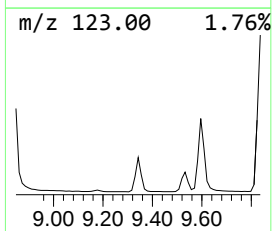
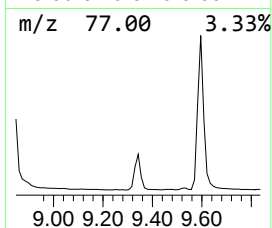
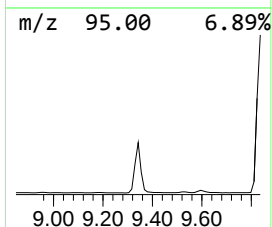
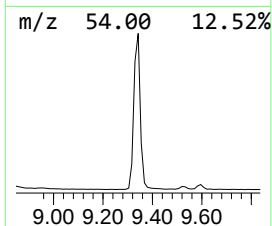
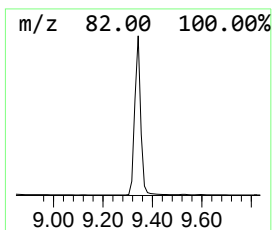
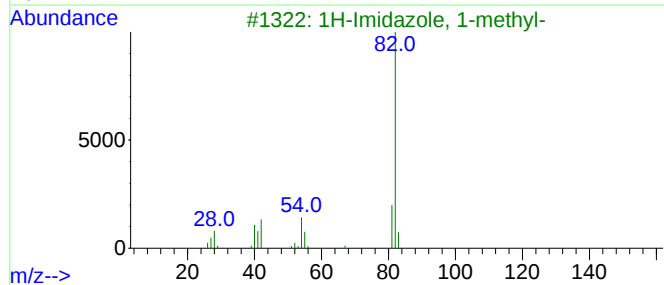
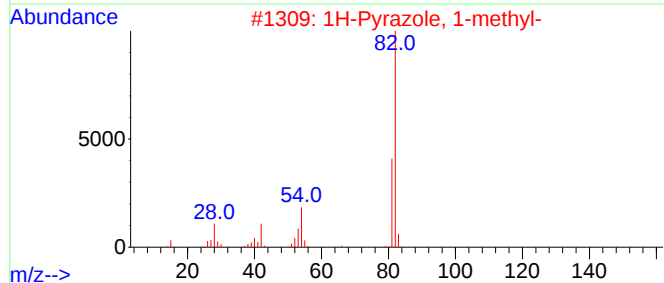
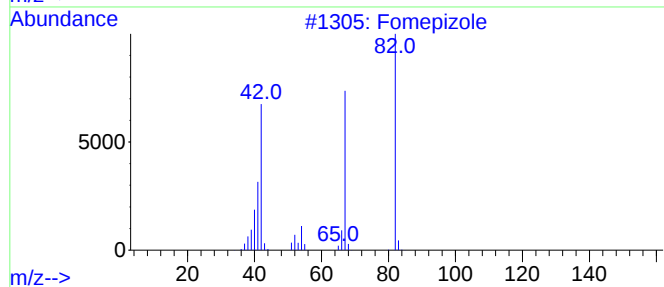
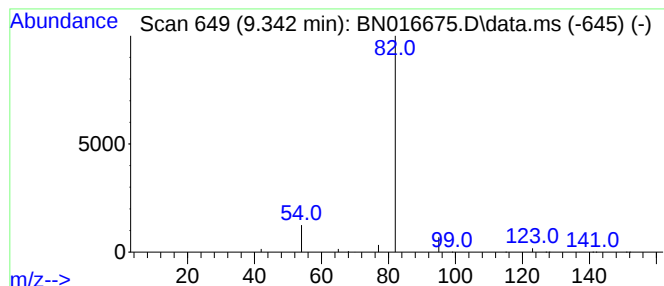
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Fomepizole Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.342	0.16 ng	83836	Naphthalene-d8	10.407

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Fomepizole	82	C4H6N2	007554-65-6	5
2			1H-Pyrazole, 1-methyl-	82	C4H6N2	000930-36-9	4
3			1H-Imidazole, 1-methyl-	82	C4H6N2	000616-47-7	4
4			Furan, 3-methyl-	82	C5H6O	000930-27-8	4
5			Furan, 2-methyl-	82	C5H6O	000534-22-5	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016675.D
Acq On : 02 Oct 2021 17:45
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Sample : PB139275BS
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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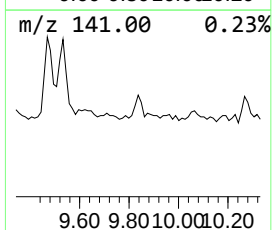
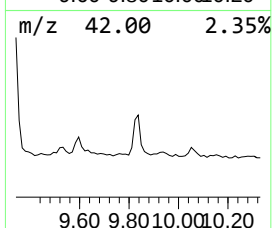
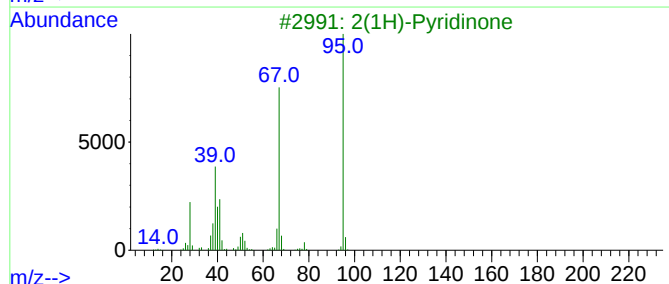
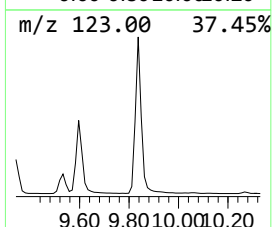
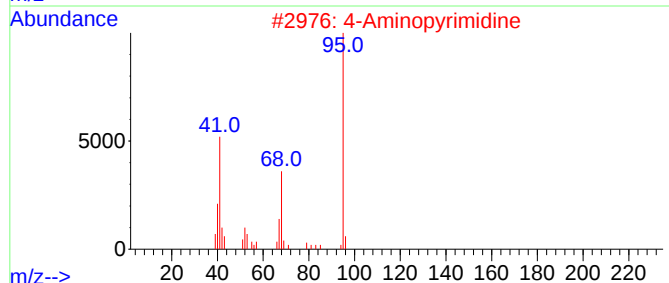
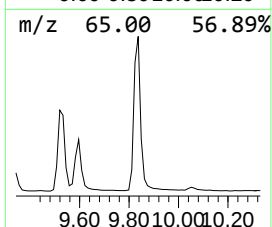
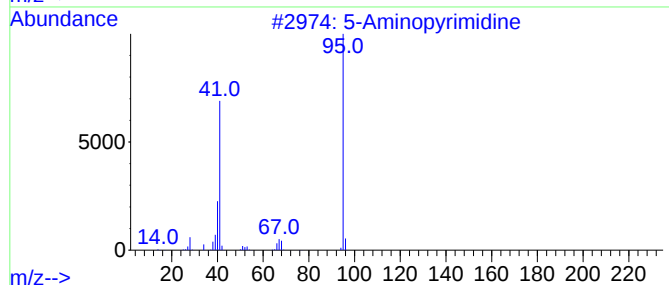
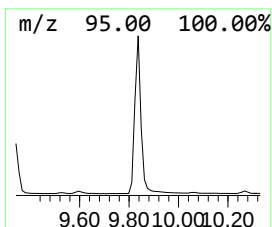
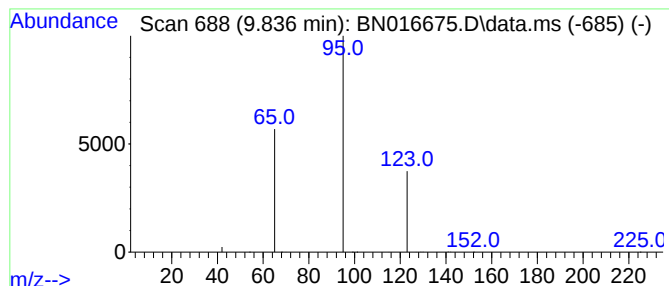
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 5-Aminopyrimidine Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.836	0.06 ng	30051	Naphthalene-d8	10.407

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Aminopyrimidine	95	C4H5N3	000591-55-9	3
2			4-Aminopyrimidine	95	C4H5N3	000591-54-8	2
3			2(1H)-Pyridinone	95	C5H5NO	000142-08-5	2
4			2-Pyrimidinamine	95	C4H5N3	000109-12-6	2
5			Pyridine, 1-oxide	95	C5H5NO	000694-59-7	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016675.D
Acq On : 02 Oct 2021 17:45
Operator : CG/JU
Sample : PB139275BS
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PB139275BS

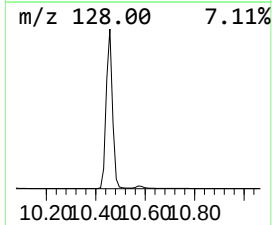
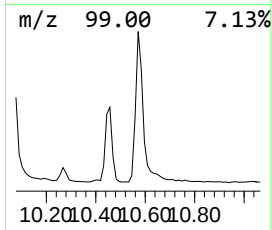
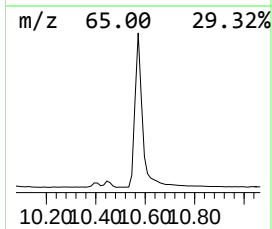
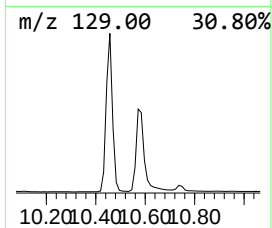
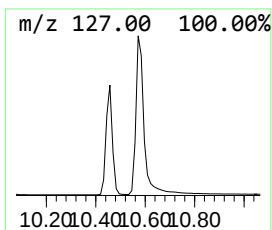
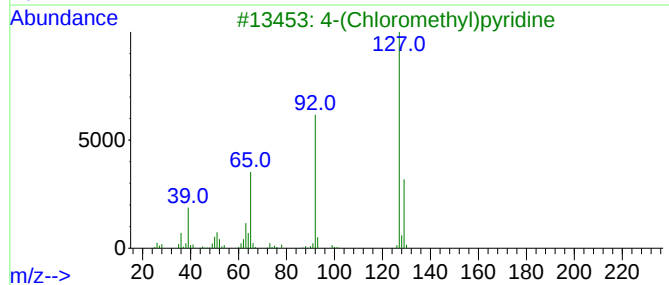
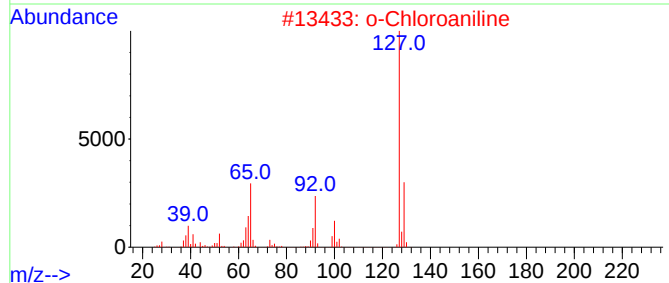
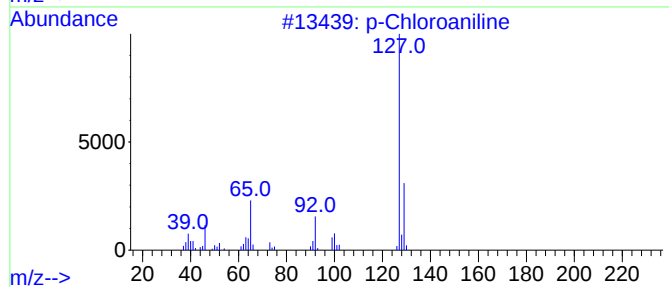
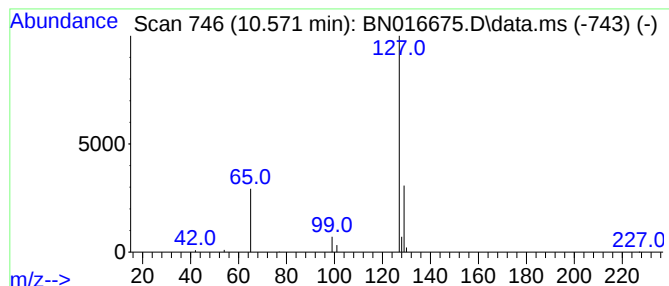
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 8 p-Chloroaniline Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.571	0.12 ng	64911	Naphthalene-d8	10.407

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			p-Chloroaniline	127	C6H6ClN	000106-47-8	90
2			o-Chloroaniline	127	C6H6ClN	000095-51-2	90
3			4-(Chloromethyl)pyridine	127	C6H6ClN	010445-91-7	90
4			m-Chloroaniline	127	C6H6ClN	000108-42-9	90
5			Picloxydine	474	C20H24Cl2N10	005636-92-0	83



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016675.D
Acq On : 02 Oct 2021 17:45
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Sample : PB139275BS
Misc :
ALS Vial : 43 Sample Multiplier: 1

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ClientSampleId :
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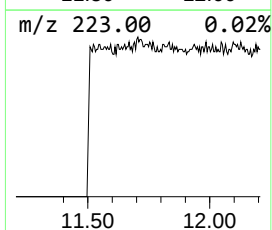
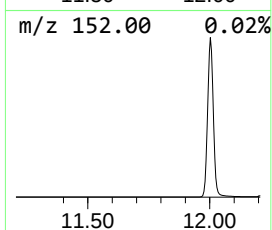
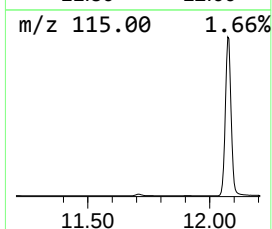
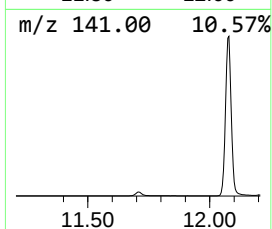
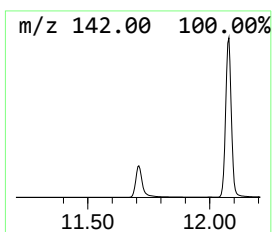
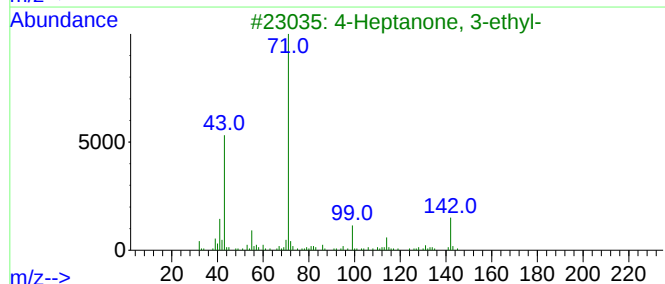
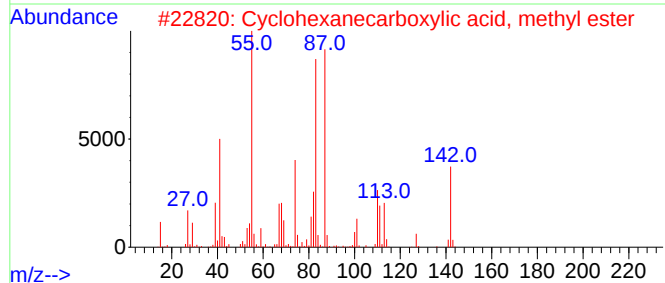
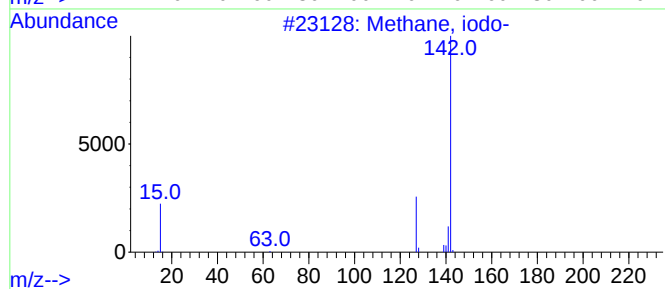
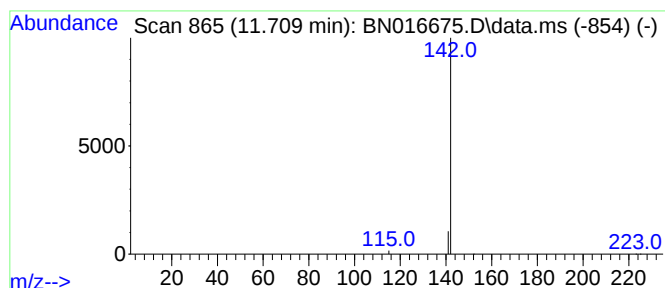
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Methane, iodo- Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.709	0.05 ng	26263	Naphthalene-d8	10.407

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methane, iodo-	142	CH3I	000074-88-4	4
2			Cyclohexanecarboxylic acid, meth...	142	C8H14O2	004630-82-4	4
3			4-Heptanone, 3-ethyl-	142	C9H18O	001528-25-2	3
4			Cyclohexane carboxylic acid hydr...	142	C7H14N2O	038941-47-8	3
5			2-Butanone, diethylhydrazone	142	C8H18N2	028236-94-4	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
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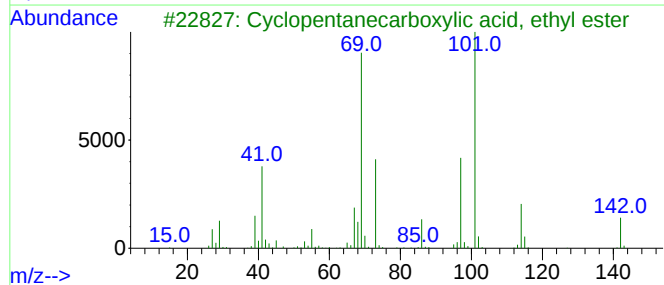
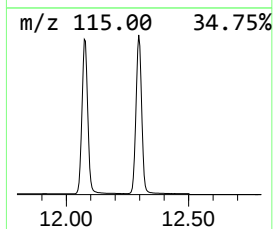
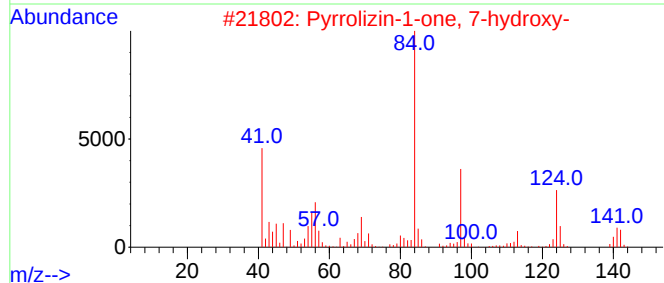
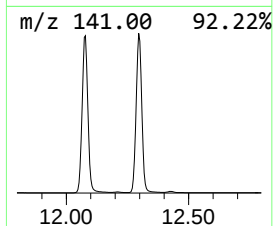
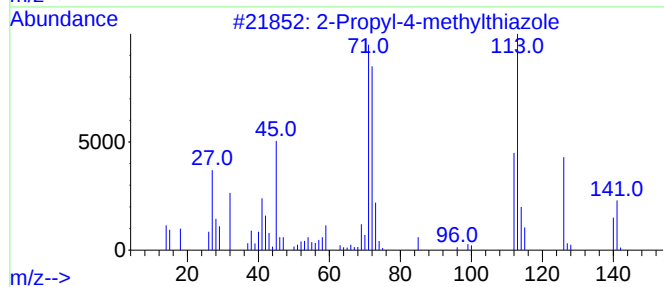
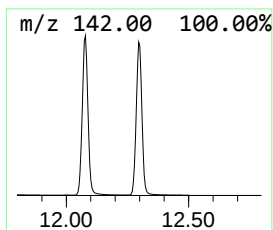
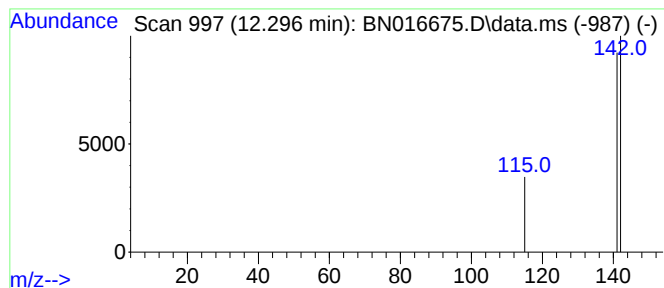
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 2-Propyl-4-methylthiazole Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.296	0.41 ng	211941	Naphthalene-d8	10.407

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Propyl-4-methylthiazole	141	C7H11NS	052414-87-6	4
2			Pyrrolizin-1-one, 7-hydroxy-	141	C7H11NO2	1000125-96-2	3
3			Cyclopentanecarboxylic acid, eth...	142	C8H14O2	1000375-86-4	3
4			2-Propionylthiazole	141	C6H7NOS	043039-98-1	3
5			2,4(1H,3H)-Pyrimidinedione, 6-am...	141	C5H7N3O2	002434-53-9	2



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ClientSampleId :
PB139275BS

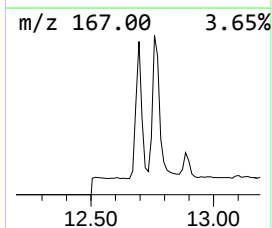
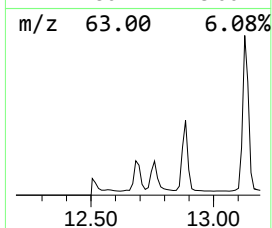
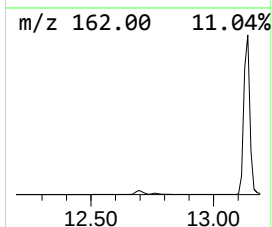
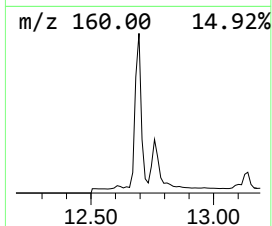
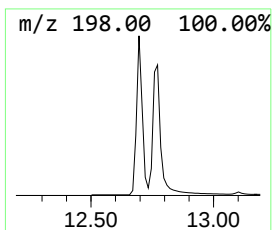
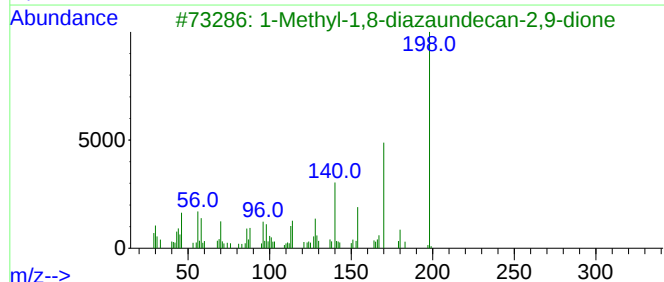
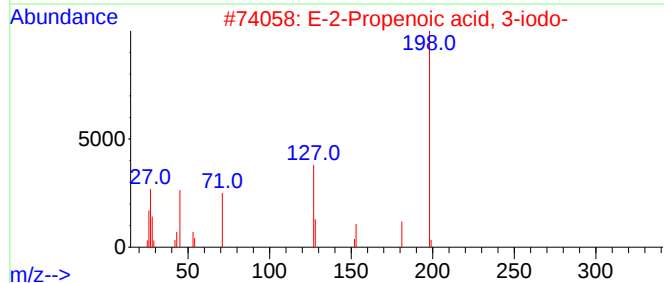
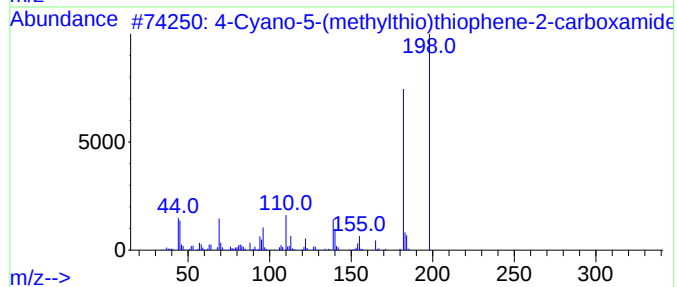
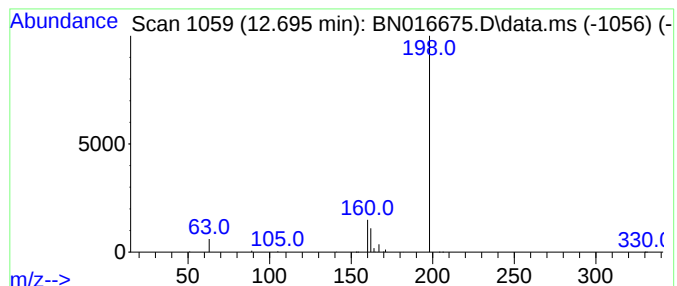
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 4-Cyano-5-(methylthio)thiop... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.695	0.06 ng	29290	Acenaphthene-d10	14.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Cyano-5-(methylthio)thiophene-...	198	C7H6N2OS2	1000267-39-2	3
2			E-2-Propenoic acid, 3-iodo-	198	C3H3IO2	1000308-86-7	3
3			1-Methyl-1,8-diazaundecan-2,9-dione	198	C10H18N2O2	1000298-94-5	3
4			Z-2-Propenoic acid, 3-iodo-	198	C3H3IO2	1000308-86-8	3
5			Thiazolo[5,4-d]pyrimidine, 5-ami...	198	C6H6N4S2	019835-31-5	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016675.D
Acq On : 02 Oct 2021 17:45
Operator : CG/JU
Sample : PB139275BS
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139275BS

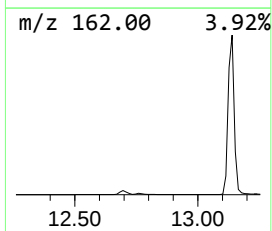
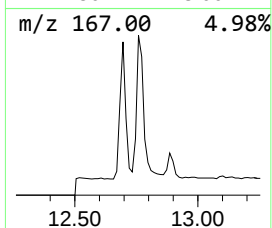
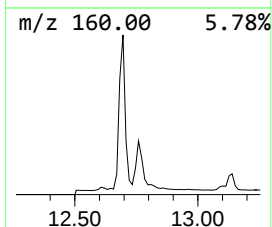
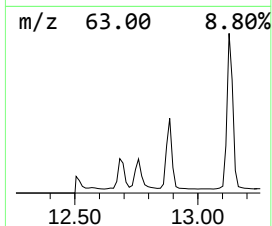
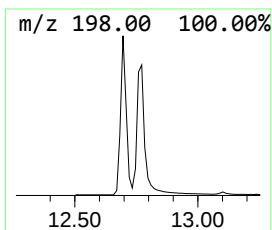
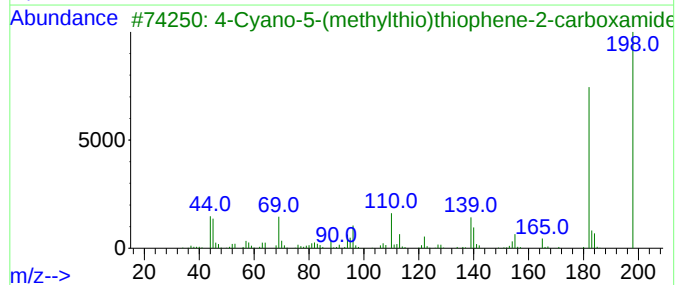
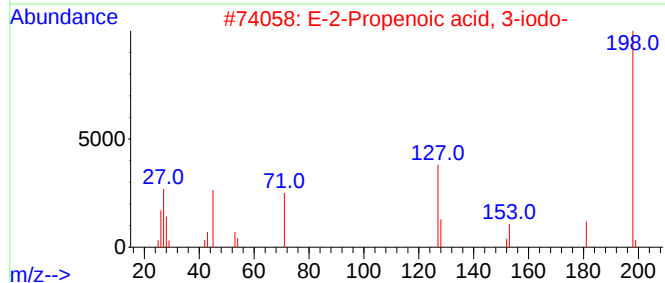
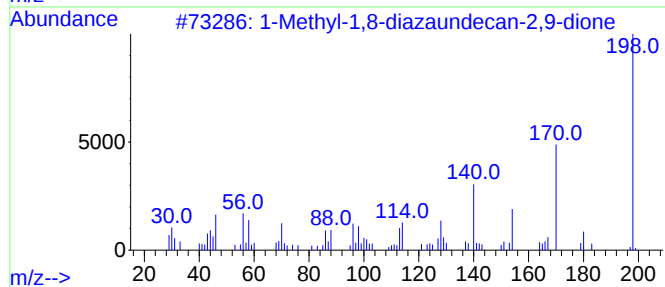
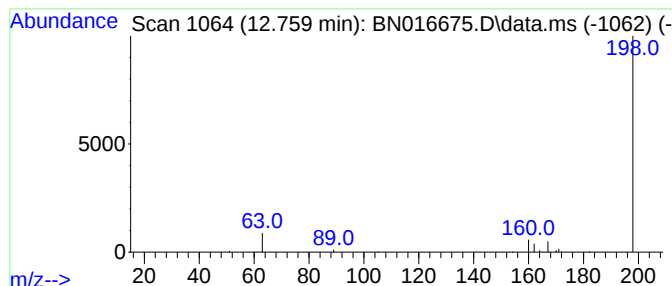
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 1-Methyl-1,8-diazaundecan-2... Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.759	0.05 ng	25220	Acenaphthene-d10	14.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Methyl-1,8-diazaundecan-2,9-dione	198	C10H18N2O2	1000298-94-5	4
2			E-2-Propenoic acid, 3-iodo-	198	C3H3IO2	1000308-86-7	3
3			4-Cyano-5-(methylthio)thiophene-...	198	C7H6N2OS2	1000267-39-2	3
4			Thiazolo[5,4-d]pyrimidine, 5-ami...	198	C6H6N4S2	019835-31-5	3
5			Z-2-Propenoic acid, 3-iodo-	198	C3H3IO2	1000308-86-8	3



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016675.D
Acq On : 02 Oct 2021 17:45
Operator : CG/JU
Sample : PB139275BS
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139275BS

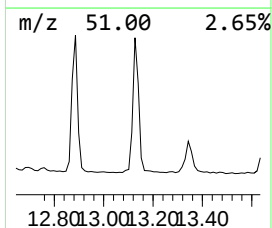
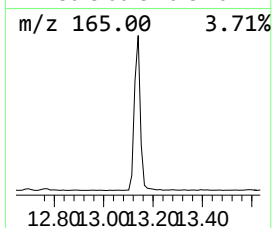
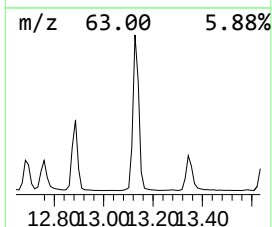
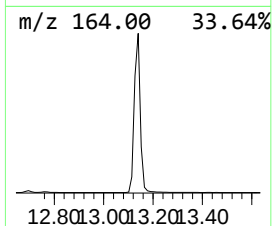
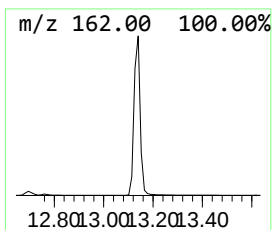
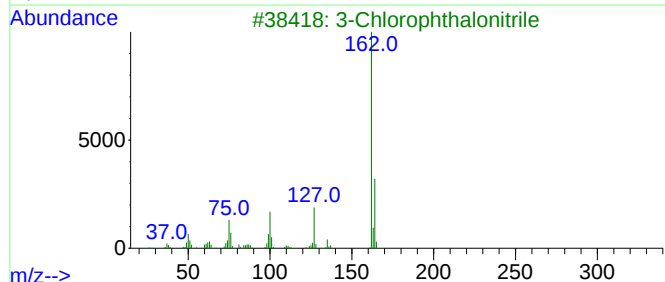
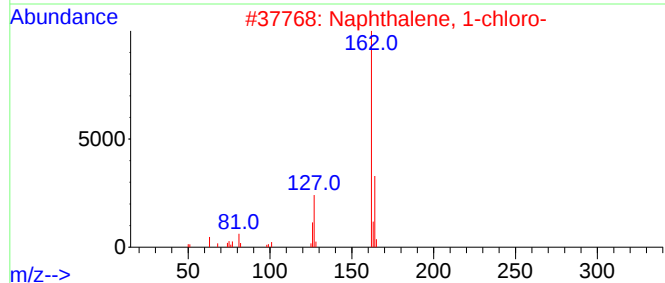
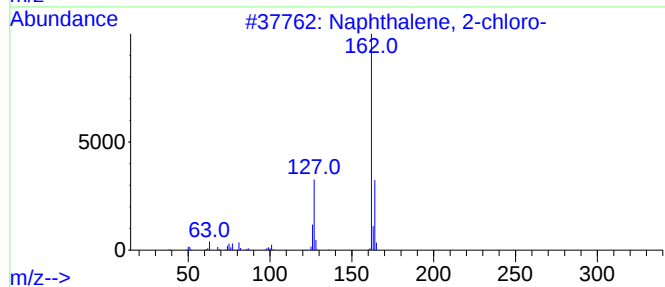
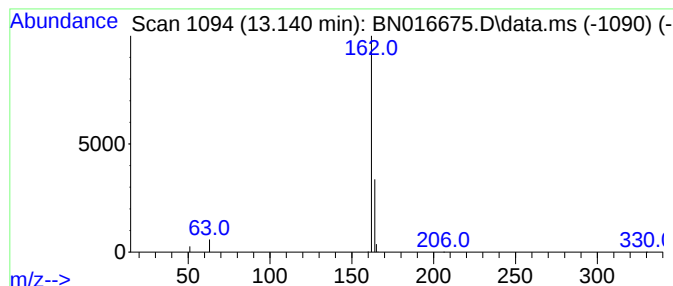
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 Naphthalene, 2-chloro- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.140	0.26 ng	135698	Acenaphthene-d10	14.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-chloro-	162	C10H7Cl	000091-58-7	74
2			Naphthalene, 1-chloro-	162	C10H7Cl	000090-13-1	74
3			3-Chlorophthalonitrile	162	C8H3ClN2	076241-79-7	7
4			2-Chloroisophthalonitrile	162	C8H3ClN2	028442-78-6	7
5			2-Amino-4-chloro-1,3-thiazole-5-...	162	C4H3ClN2OS	076874-79-8	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016675.D
Acq On : 02 Oct 2021 17:45
Operator : CG/JU
Sample : PB139275BS
Misc :
ALS Vial : 43 Sample Multiplier: 1

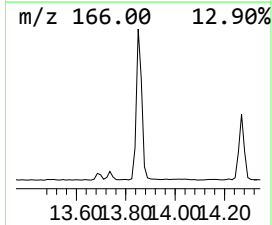
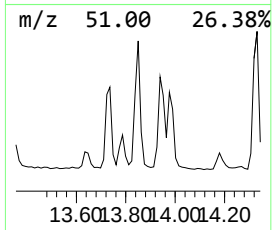
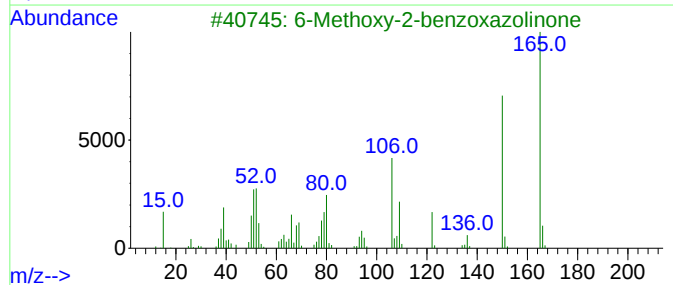
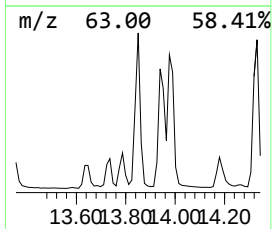
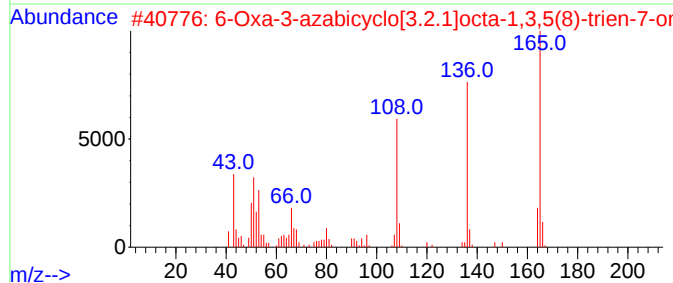
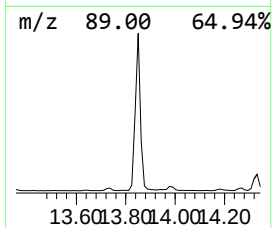
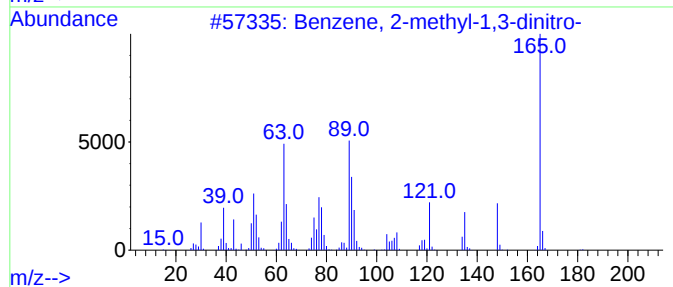
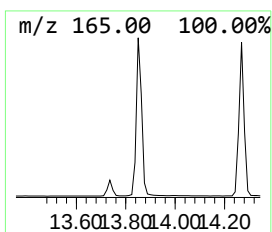
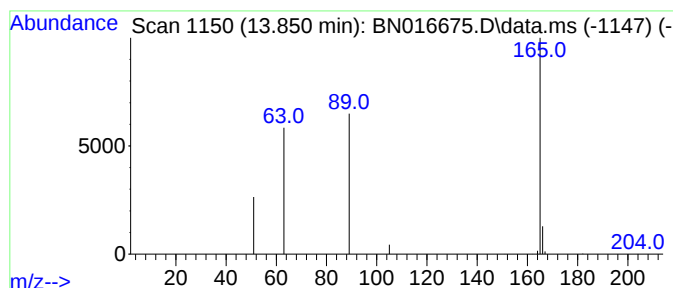
Instrument :
BNA_N
ClientSampleId :
PB139275BS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 14 Benzene, 2-methyl-1,3-dinitro- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.850	0.06 ng	28464	Acenaphthene-d10		14.269	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Benzene, 2-methyl-1,3-dinitro-		182	C7H6N2O4	000606-20-2	83
2	6-Oxa-3-azabicyclo[3.2.1]octa-1,...		165	C8H7NO3	055255-96-4	9
3	6-Methoxy-2-benzoxazolinone		165	C8H7NO3	000532-91-2	9
4	Furo[3,4-c]pyridin-3(1H)-one, 7-...		165	C8H7NO3	004543-56-0	9
5	5,6-Dimethoxy-3-pyridazinecarbon...		165	C7H7N3O2	020552-46-9	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016675.D
Acq On : 02 Oct 2021 17:45
Operator : CG/JU
Sample : PB139275BS
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
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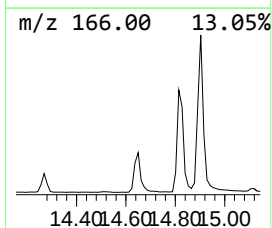
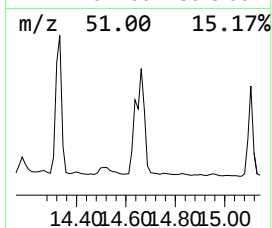
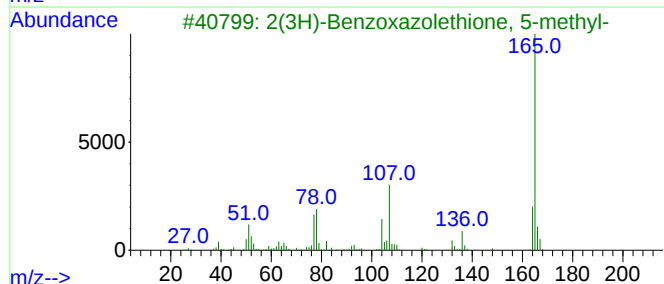
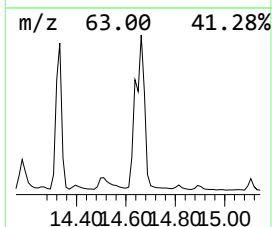
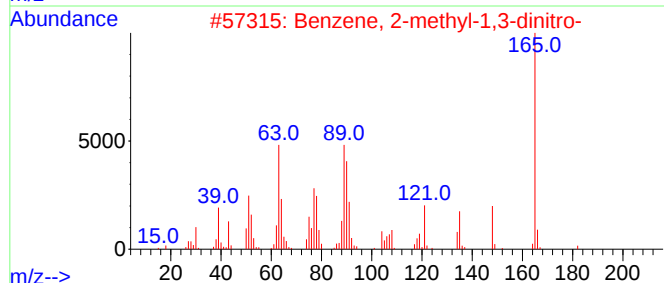
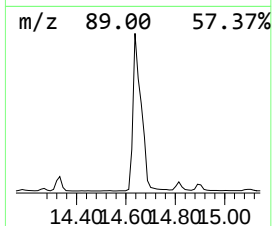
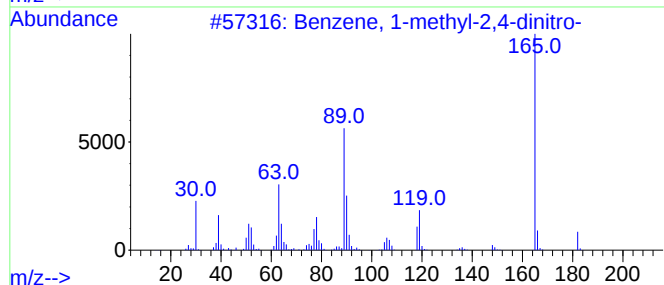
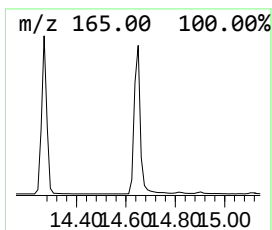
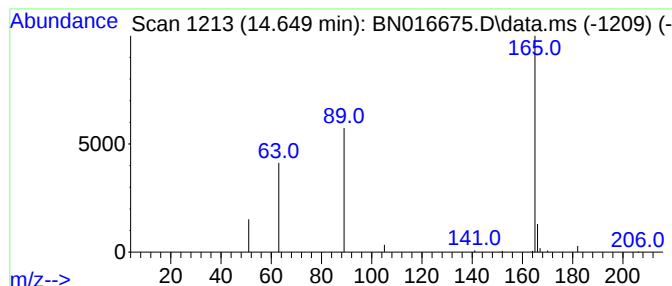
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 Benzene, 1-methyl-2,4-dinitro- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.649	0.09 ng	44123	Acenaphthene-d10	14.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-2,4-dinitro-	182	C7H6N2O4	000121-14-2	64
2			Benzene, 2-methyl-1,3-dinitro-	182	C7H6N2O4	000606-20-2	12
3			2(3H)-Benzoxazolethione, 5-methyl-	165	C8H7NOS	022876-22-8	9
4			Ethanol, 1-(4-nitrophenyl)-2-[1-...	304	C17H24N2O3	1000264-75-7	9
5			2-Chloromethyl-1,3-dichloro-2-me...	174	C5H9Cl3	001067-09-0	9



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016675.D
Acq On : 02 Oct 2021 17:45
Operator : CG/JU
Sample : PB139275BS
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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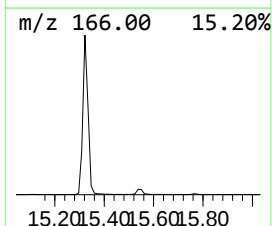
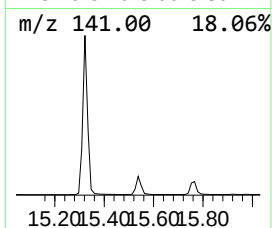
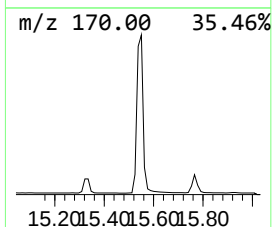
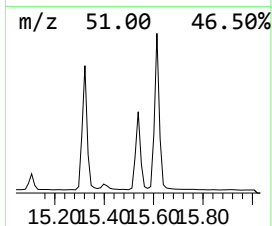
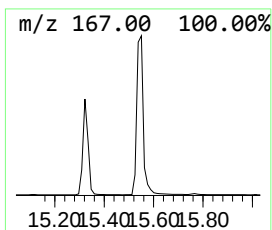
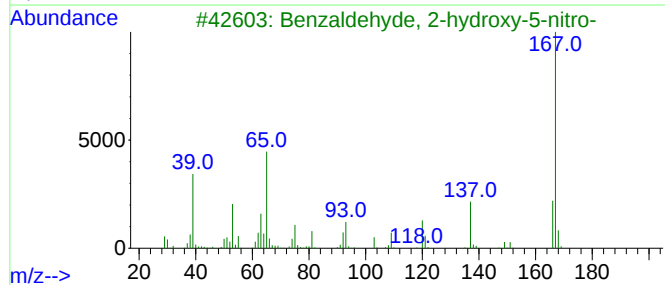
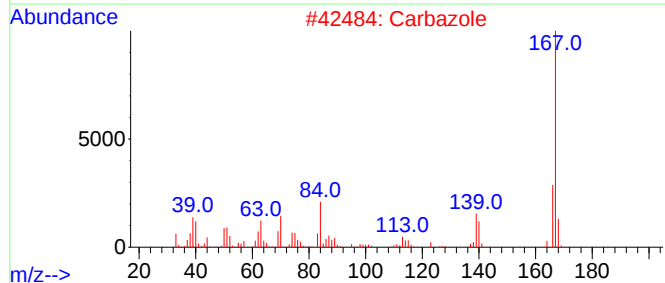
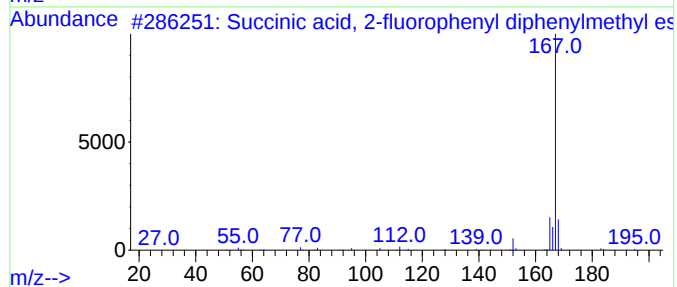
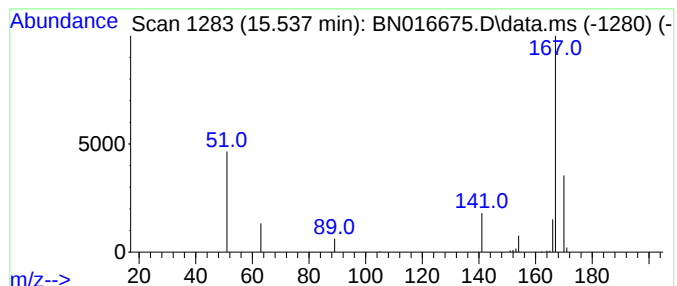
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 Succinic acid, 2-fluorophen... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.538	0.13 ng	64847	Acenaphthene-d10	14.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Succinic acid, 2-fluorophenyl di...	378	C23H19FO4	1000390-17-0	9
2			Carbazole	167	C12H9N	000086-74-8	7
3			Benzaldehyde, 2-hydroxy-5-nitro-	167	C7H5NO4	000097-51-8	5
4			5-Fluoro-2-methyl-benzothiazole	167	C8H6FNS	000399-75-7	5
5			2-Chloro-6-methylphenyl isocyanate	167	C8H6ClNO	019241-34-0	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016675.D
Acq On : 02 Oct 2021 17:45
Operator : CG/JU
Sample : PB139275BS
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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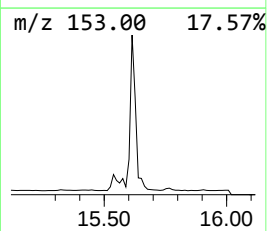
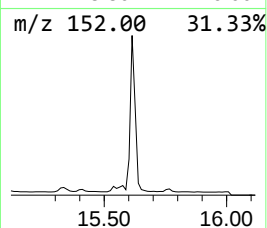
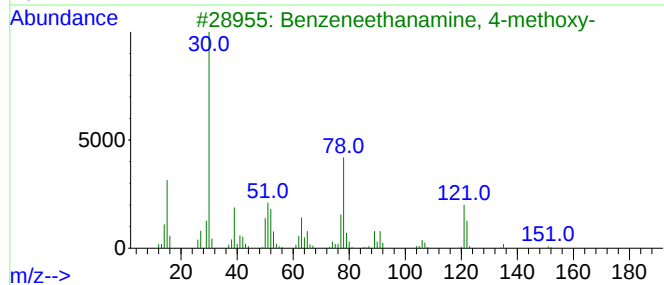
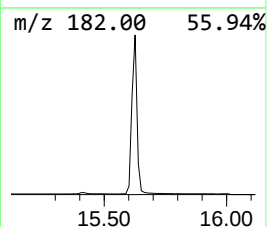
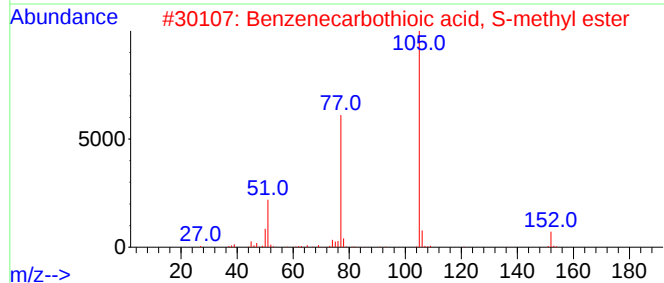
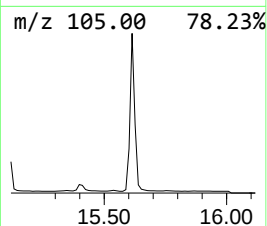
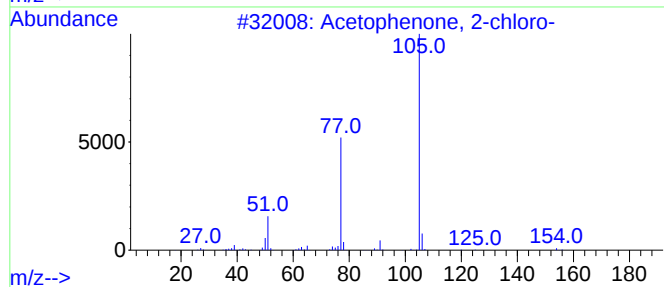
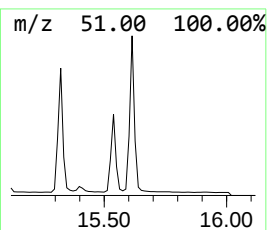
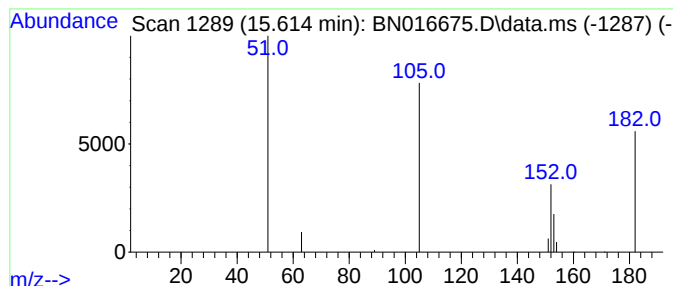
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 17 Acetophenone, 2-chloro- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.614	0.13 ng	66502	Acenaphthene-d10	14.269

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	3
2			Benzenecarbothioic acid, S-methy...	152	C8H8OS	005925-68-8	3
3			Benzenethanamine, 4-methoxy-	151	C9H13NO	000055-81-2	3
4			Propionitrile	51	C3HN	001070-71-9	3
5			Propanal, 2-(benzoyloxy)-, (R)-	178	C10H10O3	078871-04-2	2



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016675.D
Acq On : 02 Oct 2021 17:45
Operator : CG/JU
Sample : PB139275BS
Misc :
ALS Vial : 43 Sample Multiplier: 1

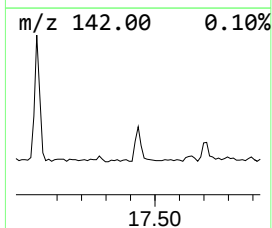
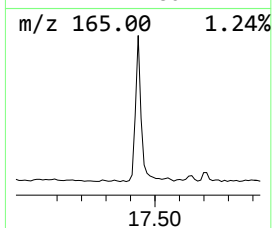
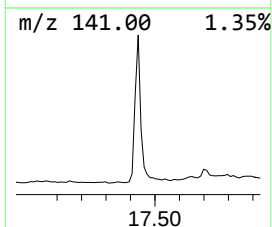
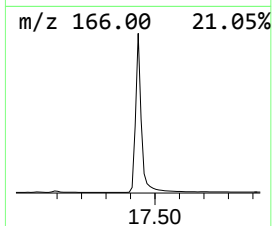
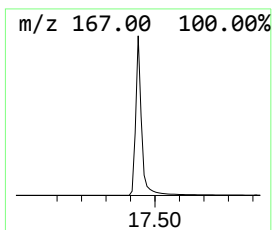
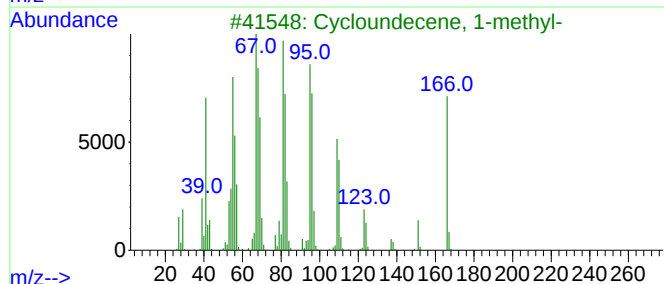
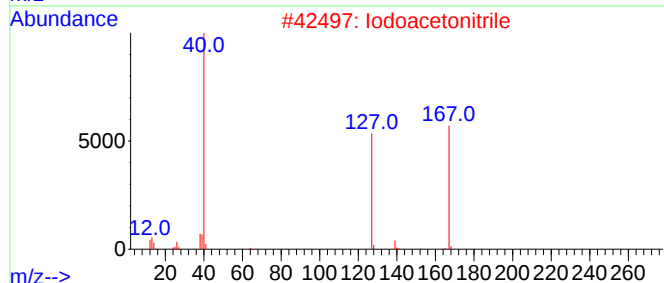
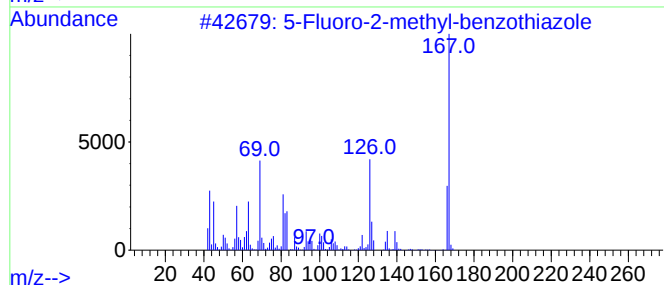
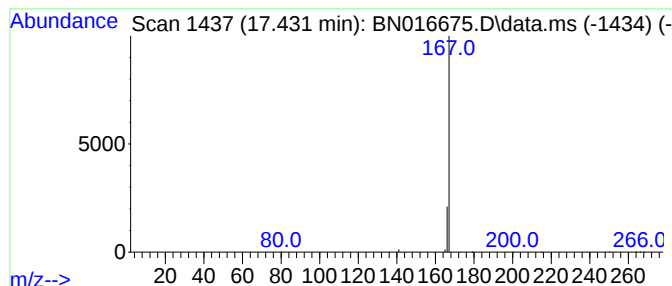
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BNA_N
ClientSampleId :
PB139275BS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 18 5-Fluoro-2-methyl-benzothia... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
17.431	0.34 ng	139873	Phenanthrene-d10		17.017	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	5-Fluoro-2-methyl-benzothiazole		167	C8H6FNS	000399-75-7	5
2	Iodoacetoneitrile		167	C2H2IN	000624-75-9	4
3	Cycloundecene, 1-methyl-		166	C12H22	088828-82-4	4
4	1,3,5-Triazine-2,4-diamine, N,N'...		167	C7H13N5	004150-59-8	4
5	1-Cyclopropanecarbonylpiperidin-...		167	C9H13NO2	063463-43-4	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016675.D
Acq On : 02 Oct 2021 17:45
Operator : CG/JU
Sample : PB139275BS
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139275BS

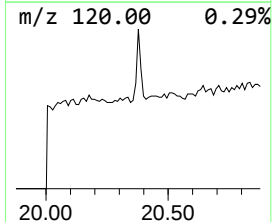
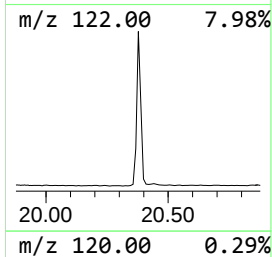
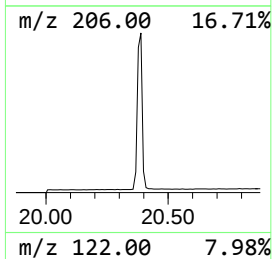
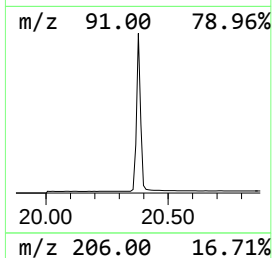
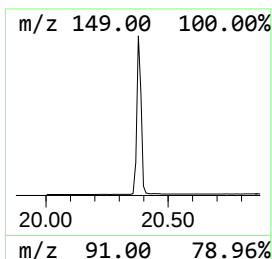
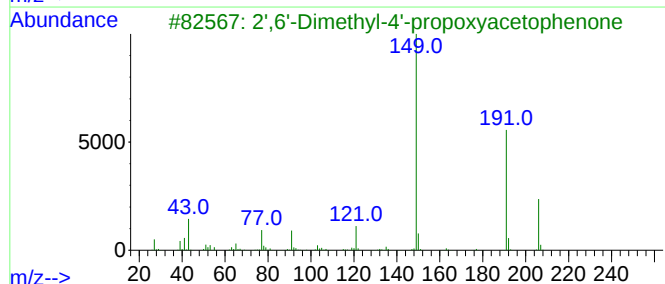
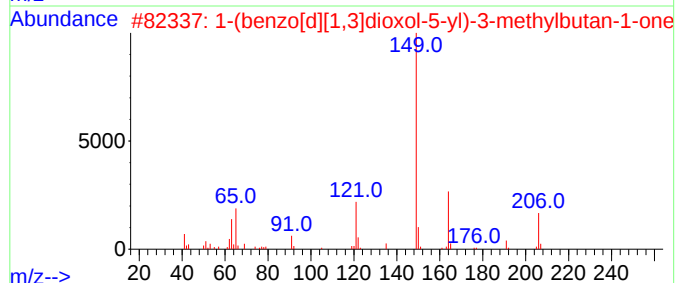
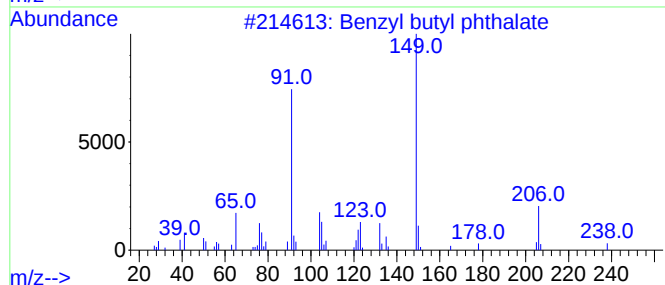
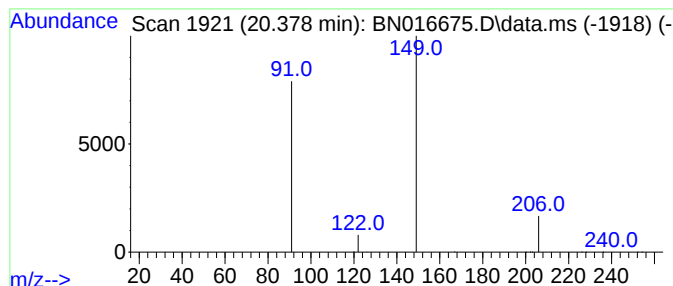
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 19 Benzyl butyl phthalate Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.378	0.05 ng	58835	Chrysene-d12	21.238

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzyl butyl phthalate	312	C19H20O4	000085-68-7	43
2			1-(benzo[d][1,3]dioxol-5-yl)-3-m...	206	C12H14O3	1000456-66-2	9
3			2',6'-Dimethyl-4'-propoxyacetoph...	206	C13H18O2	1010195-98-1	5
4			2-tert-Butyl-6-methylphenol, n-p...	206	C14H22O	1000395-19-2	5
5			1,3,2-Dioxarsenane, 2-butyl-	206	C7H15AsO2	042541-33-3	5



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
Data File : BN016675.D
Acq On : 02 Oct 2021 17:45
Operator : CG/JU
Sample : PB139275BS
Misc :
ALS Vial : 43 Sample Multiplier: 1

Instrument :
BNA_N
ClientSampleId :
PB139275BS

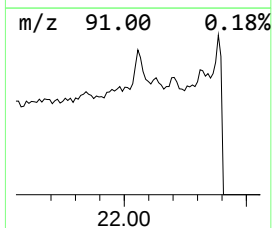
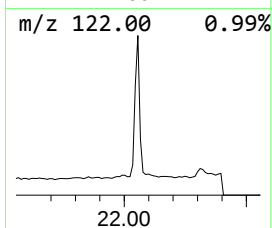
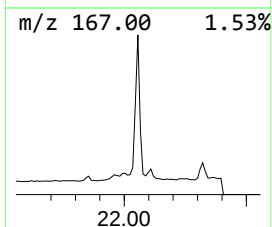
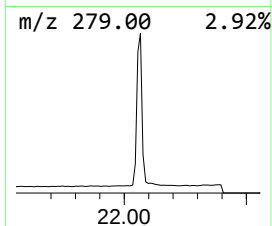
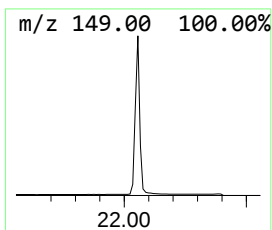
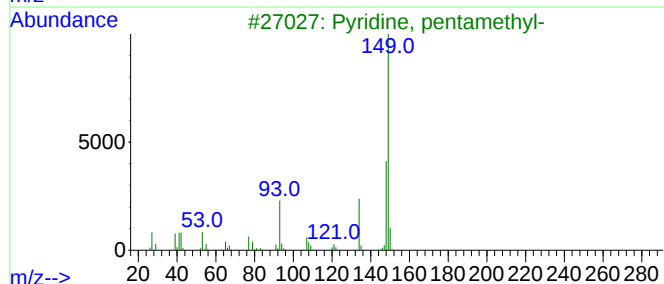
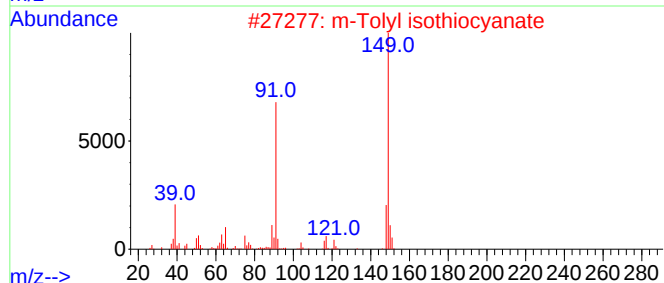
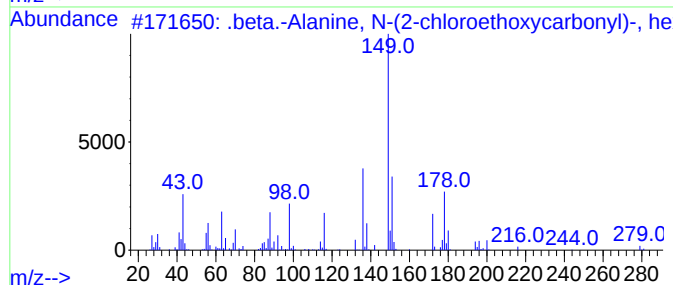
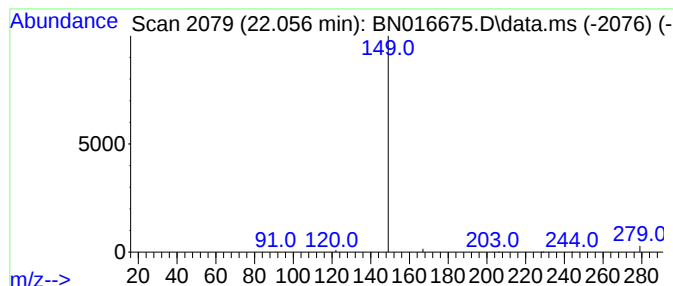
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 20 .beta.-Alanine, N-(2-chloro... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.056	0.08 ng	88945	Chrysene-d12	21.238

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		.beta.-Alanine, N-(2-chloroethox...	279	C12H22ClNO4	1010328-58-4	4
2		m-Tolyl isothiocyanate	149	C8H7NS	000621-30-7	4
3		Pyridine, pentamethyl-	149	C10H15N	003748-83-2	4
4		Phthalic acid, 7-bromoheptyl oct...	454	C23H35BrO4	1000415-52-2	4
5		Benzene, 1-isothiocyanato-4-methyl-	149	C8H7NS	000622-59-3	4



Data Path : Z:\svoasrv\HPCHEM1\BNA_N\Data\BN100121\
 Data File : BN016675.D
 Acq On : 02 Oct 2021 17:45
 Operator : CG/JU
 Sample : PB139275BS
 Misc :
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 BNA_N
 ClientSampleId :
 PB139275BS

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_N\METHODS\8270-SIM-BN100121.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST0.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Propanamine, ...	6.978	0.1	ng	39738	1	7.642	129822	0.4
Ethene, 1,1-dif...	7.200	0.1	ng	35187	1	7.642	129822	0.4
Thietane	7.523	0.1	ng	16381	1	7.642	129822	0.4
6-Benzothiazola...	7.956	0.4	ng	116882	1	7.642	129822	0.4
Furan, 2,5-dihy...	8.430	0.2	ng	53461	1	7.642	129822	0.4
Fomepizole	9.342	0.2	ng	83836	2	10.407	208631	0.4
5-Aminopyrimidine	9.836	0.1	ng	30051	2	10.407	208631	0.4
p-Chloroaniline	10.571	0.1	ng	64911	2	10.407	208631	0.4
Methane, iodo-	11.709	0.1	ng	26263	2	10.407	208631	0.4
2-Propyl-4-meth...	12.296	0.4	ng	211941	2	10.407	208631	0.4
4-Cyano-5-(meth...	12.695	0.1	ng	29290	3	14.269	206180	0.4
1-Methyl-1,8-di...	12.759	0.0	ng	25220	3	14.269	206180	0.4
Naphthalene, 2-...	13.140	0.3	ng	135698	3	14.269	206180	0.4
Benzene, 2-meth...	13.850	0.1	ng	28464	3	14.269	206180	0.4
Benzene, 1-meth...	14.649	0.1	ng	44123	3	14.269	206180	0.4
Succinic acid, ...	15.538	0.1	ng	64847	3	14.269	206180	0.4
Acetophenone, 2...	15.614	0.1	ng	66502	3	14.269	206180	0.4
5-Fluoro-2-meth...	17.431	0.3	ng	139873	4	17.017	165911	0.4
Benzyl butyl ph...	20.378	0.1	ng	58835	5	21.238	429153	0.4
.beta.-Alanine,...	22.056	0.1	ng	88945	5	21.238	429153	0.4